

### Tutorial 3: Introduction Philips X'Pert HighScore Software

Purpose: This tutorial will take you step by step through the first level of analysis on an XRD powder pattern. The pattern has been collected from an “unknown” that you have either made or was given to you. You will open Philips X'Pert HighScore software, import a scan, run various treatment routines on the data, and compare your results with known reference data from ICDD (International Centre for Diffraction Data). This software compares patterns but does not analyze an unknown pattern.

Equipment:

Collected data file called the “unknown”  
Philips X'Pert HighScore software

Procedure:

- 1) Log into Philips MPD user
- 2) Open the Philips X'Pert HighScore software
- 3) Open File - > Open - > Class 2010, sample #1.xrdml (do not over write this file)
- 4) Change the Y axis to Linear using the left tool bar
- 5) Under the Treatment tab
  - a) Click on Determine Background
    - i. Automatically adjust the Bending factor by sliding the bar and click on Accept when the background is sufficient.
  - b) Click on Strip K-Alpha 2
    - i. Choose the Rachinger method
    - ii. K-alpha2/K-alpha1 Intensity ratio = 0.5
    - iii. Click on Strip K-alpha 2
    - iv. Save to List

If you look under Scan List in the right hand side Lists Pane you will see both the measured scan and the K-alpha 2 stripped scan. Make sure that the K-alpha 2 stripped scan is checked. Again, in the Treatment tab

- c) Click on Search Peaks
  - i. Minimum significance = 2.00
  - ii. Minimum tip width (2Th) = 0.01
  - iii. Maximum tip width (2Th) = 1.00
  - iv. Peak base width (2Th) = 2.00
  - v. Method = Minimum 2<sup>nd</sup> derivative
  - vi. Click on Search Peaks
  - vii. Click on Accept (A List Pane should appear)

Under the Lists Pane click on the peak list tab. The peaks will be listed and on the scan itself there will be lines with black “v” marks on the top. You can examine the scan and make changes (add or delete peaks) by right clicking the mouse. The K-alpha 2 peaks will show up as dotted lines. Once you are satisfied with your peak list you can continue.

- 6) Under the Analysis Tab
  - a) Click on Search-Match
    - i) Under Parameters
      - a. Data Source: Peak & Profile Data
      - b. Scoring Scheme: check either Single phase or Multiphase
      - c. Check Match Intensity
      - d. Check Demote unmatched strong
      - e. Check Allow pattern shift
      - f. Known Two Theta shift (2 The) = 0
    - ii) Under Automatic
      - a. Check Identify
      - b. Maximum no. of accepted patterns: 5
      - c. Minimum candidate score: 50
      - d. Search depth: 10
      - e. Matched lines/total lines (%): 60
      - f. Minimum new lines: 5
      - g. Minimum scale factor: 0.1
    - iii) Under Restrictions
      - a. Check none
  - b) Click on Search

The software is now searching the ICDD data base for possible pattern matches. When it is finished a list of candidates will be listed on the bottom right hand side of the screen. They will be listed in descending order according to their score. If there is a very highly scored match it might appear in the top right screen as an accepted reference pattern. Below the scan is a graph of your scan compared to the current reference pattern and also any accepted patterns.

- 7) Click on a candidate and scroll down through the list of candidates observing the graph below the scan looking for matches. If you agree that the reference match is part of your pattern click and drag it to the top accepted reference pattern position. The black “v” marks above your scan should all be gone when the pattern is completely referenced.
- 8) When finished, right click on the candidates list and remove all candidates.
- 9) Under the Reports tab
  - a) Click on Word Report
  - b) Click on Default
  - c) Save your report
  - d) Print your report